ToxMiner: Relating ToxCast bioactivity profiles to phenotypic outcomes

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Abstract

One aim of the U.S. EPA ToxCast program is to develop predictive models that use in vitro assays to screen and prioritize environmental chemicals for further evaluation of potential toxicity. One aspect of this task is the compilation, quality control and analysis of large amounts of in vitro and in vivo data to develop predictive models or signatures. We have developed a computer system called ToxMiner which combines a database and statistical analysis tools to carry out these tasks. The ToxMiner database, which is one component of the larger EPA ACToR (Aggregated Computational Toxicology Resource, http://actor.epa.gov) holds in vitro assay data generated by the ToxCast program, in vivo animal data, gathered through the EPA ToxRefDB effort (http://www.epa.gov/ncct/toxrefdb) and related biological information on genes and pathways. The ToxMiner statistical tools can find univariate associations between in vitro and in vivo data and can produce machine learning predictive signatures. We demonstrate the use of ToxMiner by showing examples of signatures for whole animal toxicity from cancer, developmental and reproductive endpoints.

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